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# **A FRAMEWORK FOR MULTISCALE MODELING OF DEFORMATION IN CRYSTALLINE SOLIDS**

**AFOSR AWARD NO. FA9550-05-1-0033**

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## **Abstract**

A simulation framework was developed for studying the deformation behavior of metallic materials. Atomistic simulations were employed to study dislocation nucleation during nanoindentation and to correlate dislocation behavior and overall material response in thin-film crystals. An instrumented indenter was acquired to study the indentation behavior of metallic composites. Experimental and continuum-based modeling works on indentation of discontinuously reinforced metal matrix composites were also conducted. Detailed microscopic features were analyzed, which aided in our fundamental understanding of plastic deformation in these materials.

## **Research Objectives**

This project is devoted to employing computational methods to simulate micro- and nano-scale dislocation plasticity in metallic crystals. Specifically, computer simulations are undertaken to probe the dislocation actions at the defect and atomistic levels. Extensive modifications of our current codes have been carried out to target problems on indentation and mechanical behavior at small length scales. The acquisition of an instrumented micro-indenter for performing experimental verification is included in this project. In this report, we document the salient achievements of our efforts as outlined below.

## **Atomistic Simulations of Nanoindentation**

Nanoindentation has received considerable attention in recent years, due in part to its practicability as an experimental means in probing surface mechanical properties of bulk

and miniaturized materials. Experiments on pure face-center-cubic crystals using load-controlled devices have shown sudden displacement excursions in the indentation load-displacement curve, which was thought to be caused by the homogeneous nucleation of dislocations. In-situ experimental simulation using the bubble-raft model has illustrated the homogeneous dislocation nucleation event in a two-dimensional (2D) crystalline array under indentation. We have carried out a computational parallel to such experimental observations using a 2D molecular statics approach.

Figure 1 shows a model 2D crystal, having the close-packed crystal structure, under circular indentation to a certain depth. Subsurface nucleation of two pairs of dislocations has occurred and they have slipped over certain distances in response to the indentation loading, as highlighted. The simulated indentation load-displacement curve displayed sudden reduction in load as a consequence of dislocation nucleation. Attempts for correlating the nucleation event with local strain fields have been made. Figures 2(a) and (b) show the simulated shear strain fields, resolved in the  $\pm 60^\circ$  directions (slip directions), right before the dislocations nucleated. The dislocation nucleation site coincides with the maximum resolved shear strain site, with a strain magnitude being approximately 0.085. Another set of simulations using a different indenter size has given a quantitatively consistent result. The critical strain value is very close to that from the classical Frenkel's approach of theoretical shear strength of crystals. The modeling framework can be extended to study the strengthening and dislocation plasticity events in nanolayered thin-film structures.

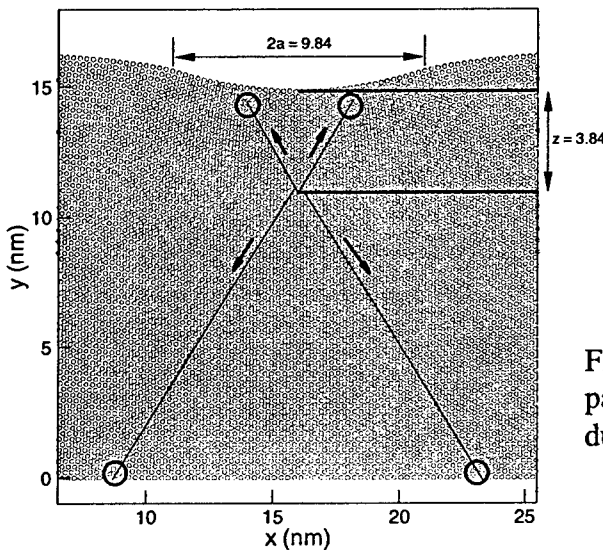


Fig. 1 Simulated nucleation of two pairs of dislocations in a model crystal during indentation loading.

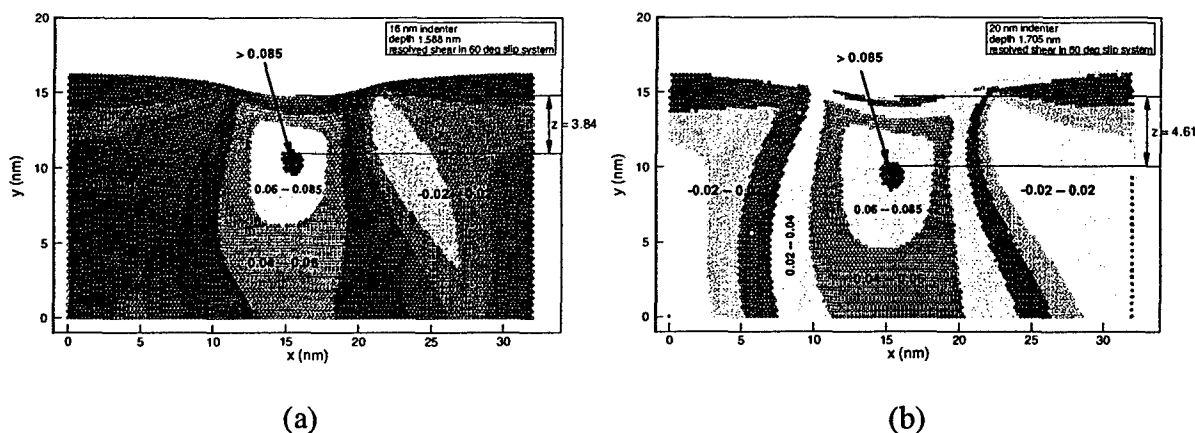
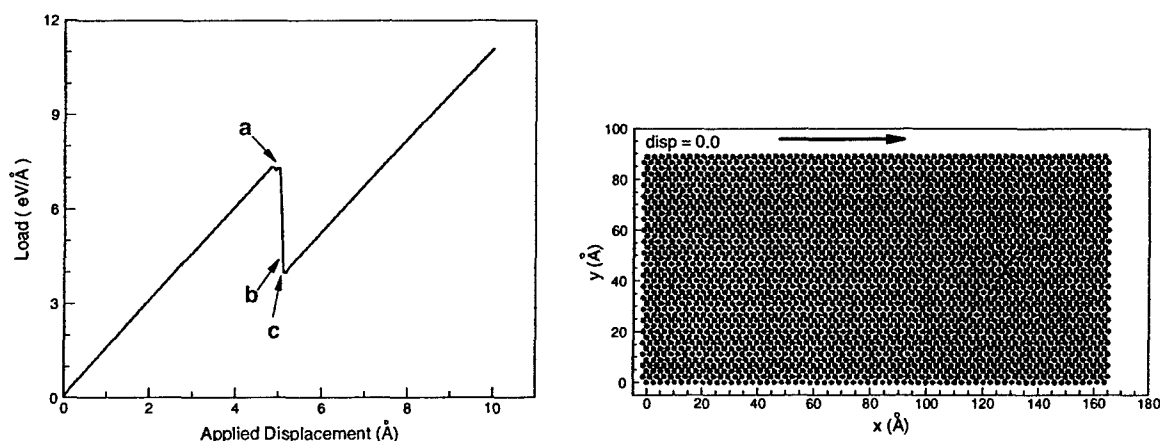


Fig. 2 Simulated shear strain contours resolved in the two slip directions right before dislocation nucleation occurs.

### Atomistic Simulations of Dislocation Plasticity

The same modeling approach was also used to study dislocation behavior in thin-film crystals under general loading conditions. To trigger dislocations in an otherwise perfect crystal for non-localized loading, a defect source is required. Here we adopted a strategy that a self-interstitial is placed inside the model and is allowed to equilibrate with its surrounding atoms before loading commences.

An example is shown in Fig. 3 where the crystal is subject to simple shear loading along the x-direction. A pair of dislocations evolves from the initial defect, as highlighted in the figure. The overall load-displacement curve shows a sudden drop in load, which is associated with the slipping of dislocations out of the crystal to create a slip step on each side, as illustrated by the atomic snapshots. A permanent shape change of the crystal thus results.



(Fig. 3, continued below)

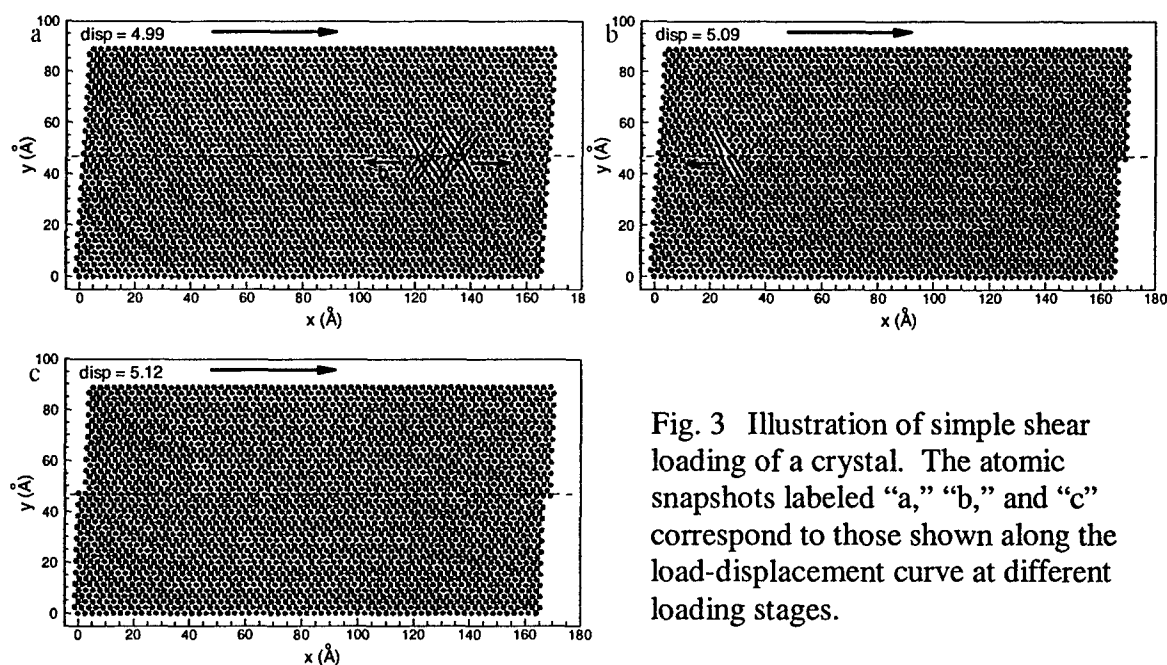


Fig. 3 Illustration of simple shear loading of a crystal. The atomic snapshots labeled “a,” “b,” and “c” correspond to those shown along the load-displacement curve at different loading stages.

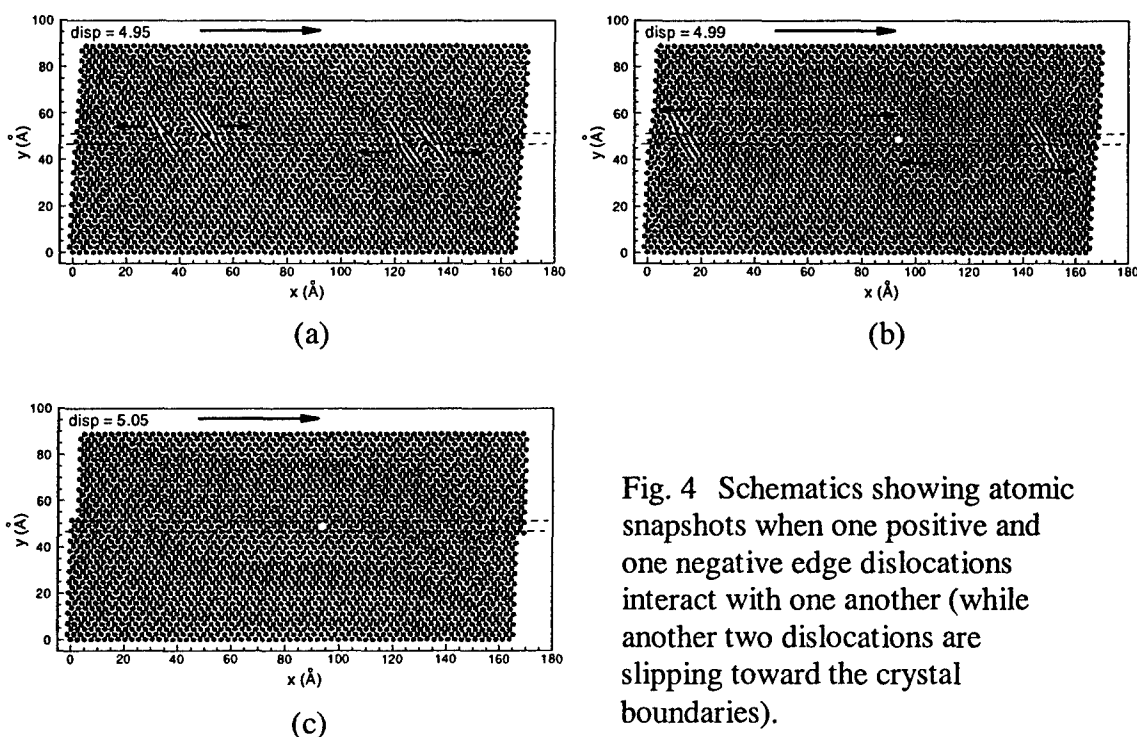


Fig. 4 Schematics showing atomic snapshots when one positive and one negative edge dislocations interact with one another (while another two dislocations are slipping toward the crystal boundaries).

We have undertaken analyses on the dislocation-dislocation interaction in the structure. Figures 4 illustrate a case for dislocation interaction leading to a point defect. In Fig. 4(a) two dislocation dipoles can be seen, with the inner dislocations approaching each other in

response to the applied shear. Because these two dislocations are gliding on different slip planes separated by one atomic layer, in Fig. 4(b) annihilation has taken place but with a vacancy left behind. In Fig. 4(c) the two outer dislocations have moved out of the crystal. A systematic analysis was performed, and the detailed results were published in Popova et al. as documented below.

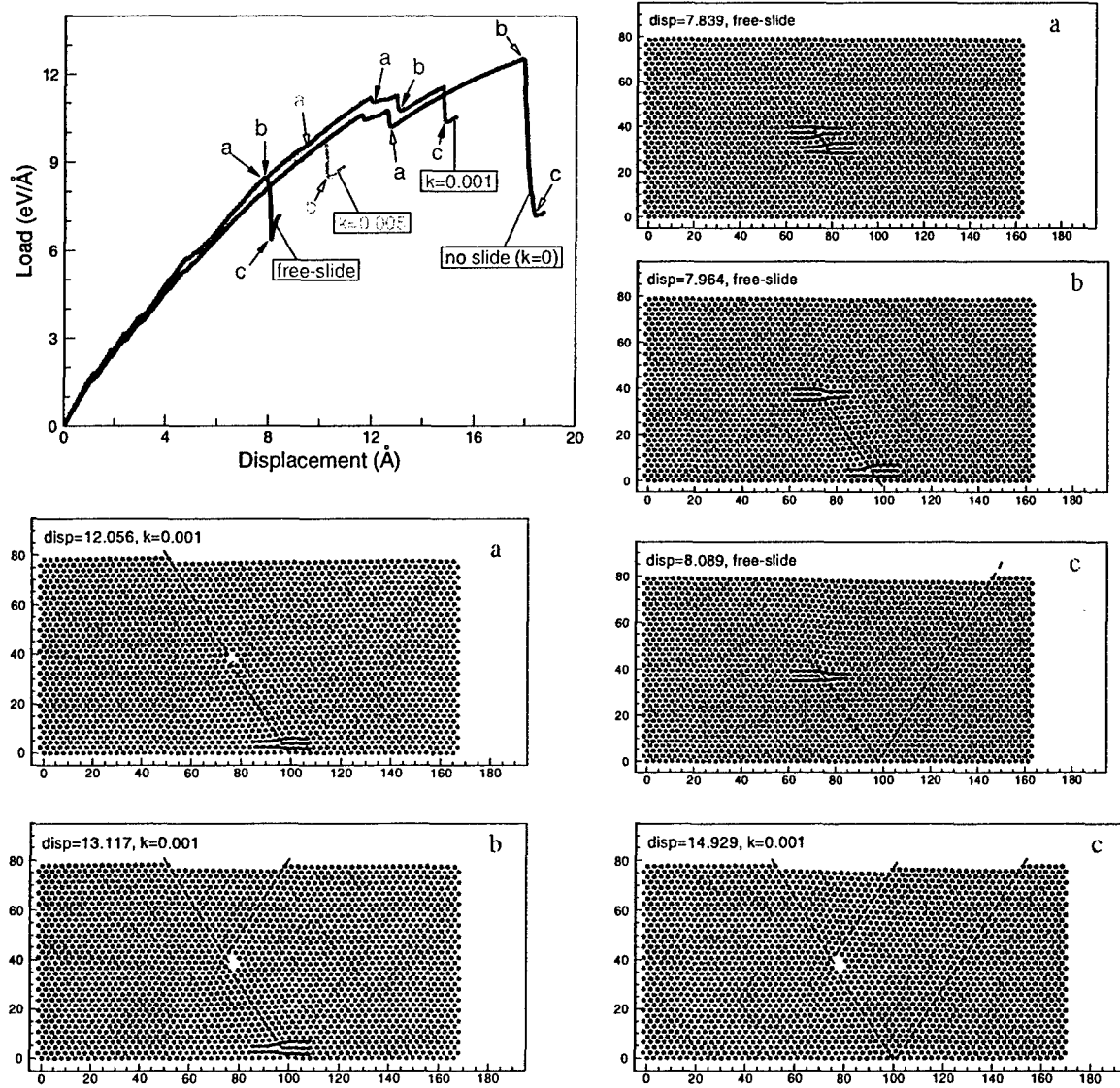


Fig. 5 Select results on dislocation-interface interactions, with controlled interface sliding features taken into consideration.

### Atomistic Simulations of Dislocation-Interface Interaction

Here we present an example of the dislocation interaction with an interface between the metal film and a stiff substrate. The loading is tensile with prescribed incremental

displacements applied on the right boundary atoms. The substrate material is not specifically accounted for. However, the atoms along the bottom boundary of the film are restricted to maintain their  $y$ -positions. Their movements along the  $x$ -direction are controlled to different extents, signifying the different interface sliding capabilities investigated. In the extreme case of no slide, the  $x$ -component displacements of interface atoms are made proportional to the prescribed boundary displacement, simulating perfect bonding with the substrate which controls the macroscopic deformation. The maximum allowable displacement along the interface, applied individually on interface atoms, is expressed as

$$u_{x,\max} = k \cdot r_{\text{int}} \quad (1)$$

where  $r_{\text{int}}$  represents the spacing between adjacent atoms along the interface at the beginning of the *current* loading increment (controlled by the prescribed boundary displacement), and  $k$  is the sliding parameter. The parameter  $k$  is henceforth used to designate the extent of sliding allowed in the model. Figure 5 shows the load-displacement curves for four different cases of interface sliding and some representative atomic snapshots of the cases of free slide and  $k = 0.001$ .

The plots in Fig. 5, with the corresponding colors and symbols shown, are largely self explanatory. The important observations are that plastic yielding of the film is more delayed with a decreasing capability of interfacial slide (with the dislocation “rebound” at the interface being more difficult to occur), and that the overall film response and the underlying dislocation behavior are extremely sensitive to the interfacial sliding characteristics. Details can be found in the paper Shen and Leger documented below.

### **Experiments on Instrumented Indentation**

Through this project we have acquired a Romulus Alexandra I instrumented indenter. The intent is to conduct experimental studies on a wide variety of metallic materials and composites. One particular focus is on the indentation response of heterogeneous materials. Here we present results with a discontinuously reinforced metal matrix composite. The material is the 2124 aluminum (Al) alloy reinforced with 13.2 vol.% silicon carbide (SiC) whiskers (short fibers), with the whiskers oriented largely along a single direction (defined as the “longitudinal” direction). Special attention is devoted to

the indentation response in two different loading directions: parallel to the whisker orientation (longitudinal) and perpendicular to the whisker orientation (defined as the “lateral” direction). Figure 6 shows a representative result of the measured Vickers hardness values under various indentation loads (25, 50, and 100 N) along the two different directions. It is interesting to note that the lateral case consistently shows higher hardness values than the longitudinal case. This is counterintuitive, since for such type of composites under typical uniaxial loading, longitudinal loading always results in higher overall strength than lateral loading.

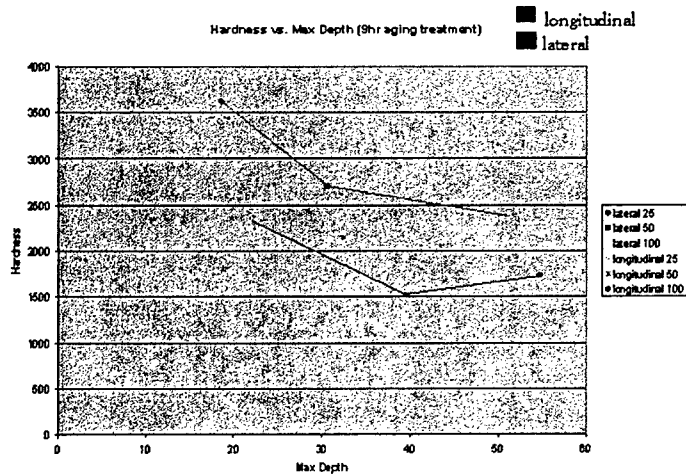


Fig. 6 Measured Vickers hardness at different loads (25 N, 50 N and 100 N), for the cases where indentation is perpendicular to (referred to as “lateral”) and parallel to (referred to as “longitudinal”) the fiber direction. The depth unit is in  $\mu\text{m}$ .

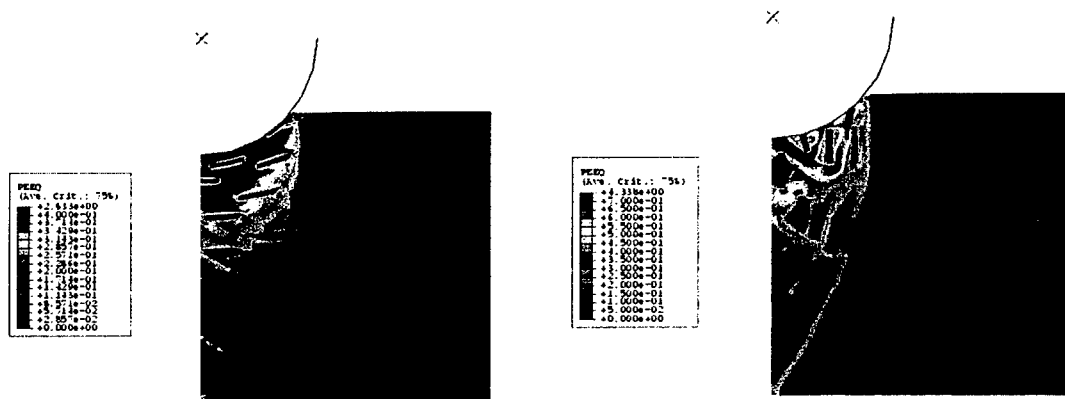


Fig. 7 Contours of equivalent plastic strains under indentation loading in the cases of (a) lateral and (b) longitudinal directions. Some whiskers are discernible near the indentation site.

Numerical simulations using the finite element method were employed to rationalize the experimental observations. The analyses utilized near random distributions of SiC whiskers embedded within the Al matrix, under the 2D plane strain condition. Some



results in the form of contour plots of equivalent plastic strains are shown in Figs. 7(a) (lateral indentation) and 7(b) (longitudinal indentation). Only the whiskers in the severely deformed region can be seen. The simulated indentation loading, shown in Fig. 8, actually shows a harder response in the lateral case than in the longitudinal case, in consistence with the experiments.

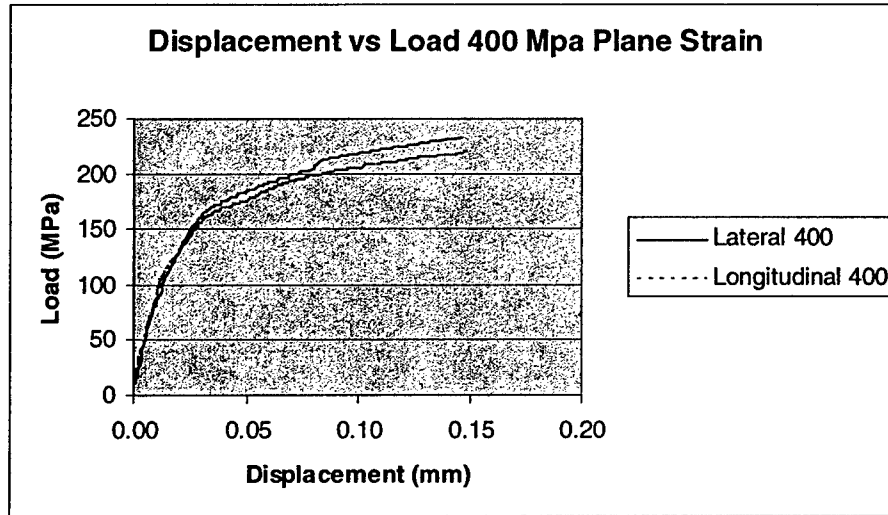


Fig. 8 Numerically simulated indentation load-displacement curves for the cases of lateral and longitudinal loading.

We have also used nanoindentation to measure the surface residual stress in SiC particle reinforced Al matrix composites. The technique features extrapolation of spherical indentation data from the post-yield regime to determine the contact radius at the onset of yielding. With the known yield strength of the matrix material, the biaxial residual stress was obtained on the basis of a closed form solution. It is found that the residual stress is primarily due to thermal expansion mismatch between Al and SiC, and the tensile stress magnitude increases with the particle volume fraction. For the composite containing 30 vol.% SiC particles, the residual stress in Al reaches 268.8 MPa, which is considerably lower than the yield strength of the unreinforced matrix. The experimental result compares favorably with numerical modeling using the finite element analysis, as illustrated in Fig. 9. Further details can be found in the publication Olivas et al. listed below.

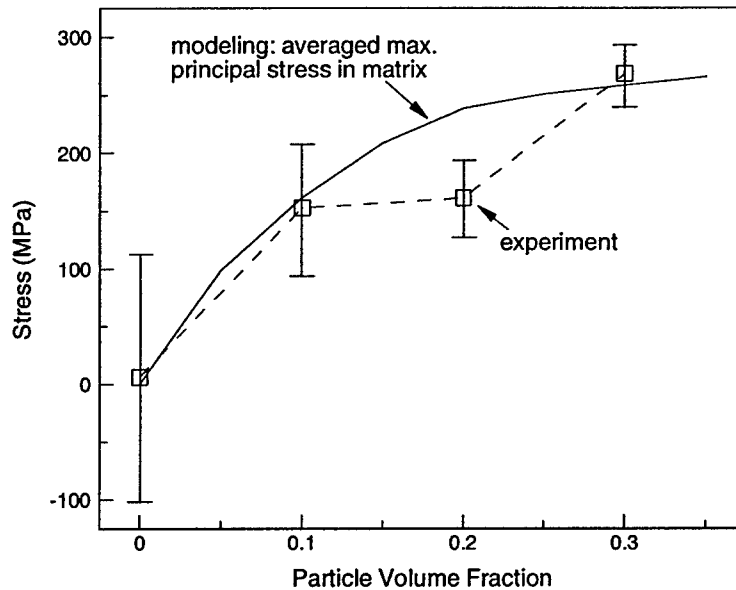


Fig. 9 Comparison of experimental nanoindentation measurement of residual stress in the matrix and the finite element modeling of averaged maximum principal stress in the matrix. The error bars for the measured data are also included.

#### Acknowledgment/Disclaimer

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#### Personnel Supported

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Yu-Lin Shen	Associate Professor, University of New Mexico
Tariq Khraishi	Assistant Professor, University of New Mexico

## **Publications**

1. M. Popova, Y.-L. Shen and T. A. Khraishi, "Atomistic Simulation of Dislocation Interactions in a Model Crystal," *Molecular Simulation*, vol. 31, pp. 1043-1049 (2005).
2. Y.-L. Shen and R. W. Leger, "Parametric Atomistic Analysis of Dislocation-Interface Interactions in Thin Metallic Films," *Materials Science and Engineering A*, in press.
3. E. R. Olivas, J. G. Swadener and Y.-L. Shen, "Nanoindentation Measurement of Surface Residual Stresses in Particle-Reinforced Metal Matrix Composites," *Scripta Materialia*, vol. 54, pp. 263-268 (2006).

## **Awards Received**

Yu-Lin Shen, Fellow of ASME, elected 2005

ANS (American Nuclear Society) 2004 Materials Science and Technology Division Literary Award. Paper titled: "Mechanical Property Degradation in Irradiated Materials: A Multiscale Modeling Approach" in *Nuclear Instruments and Methods B*. Work co-authored by Tariq Khraishi and others.